



Localization of strands in random trivial braids

Sergei Nechaev

LPTMS, CNRS & Université Paris Saclay, France

Motivation:

Puzzling numerical simulations of fluctuations in a melt of
unentangled directed polymers

by

Pablo Serna, Guy Bunin, and Adam Nahum (PRL, 2015)

Work in collaboration with:

Pieter Hendrik Willem Van Der Hoek

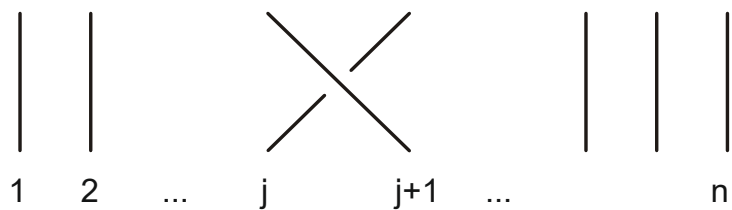
SISSA, Trieste, Italy

and

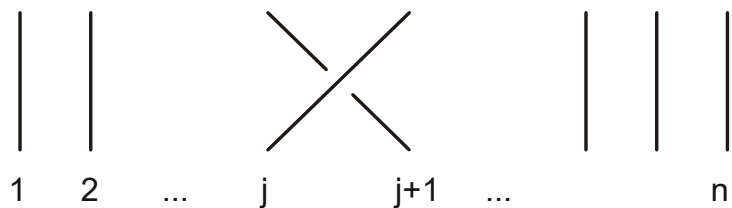
Daniil Fedotov

Universite Paris Saclay, Orsay, France

What are braids?

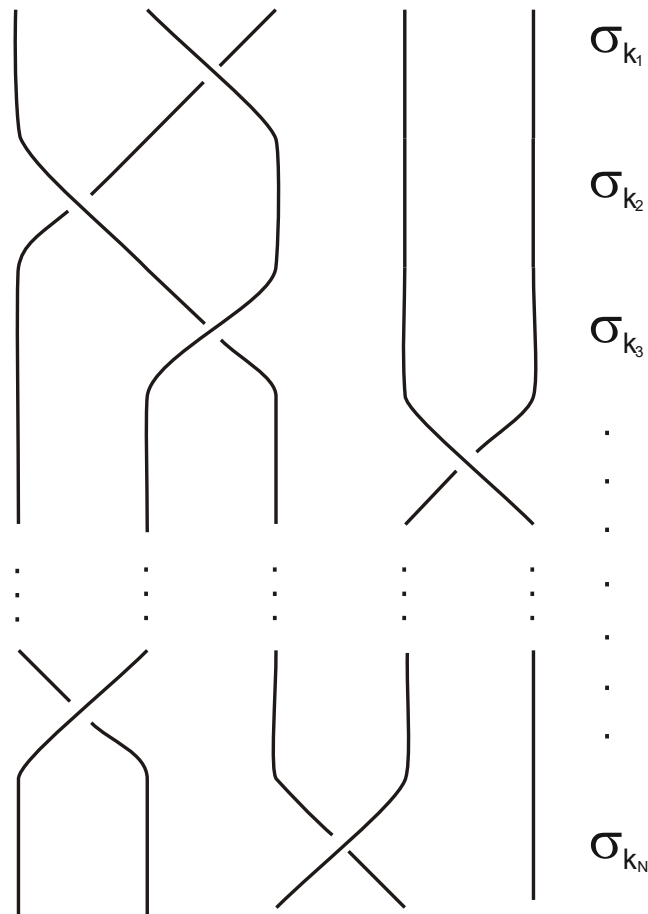
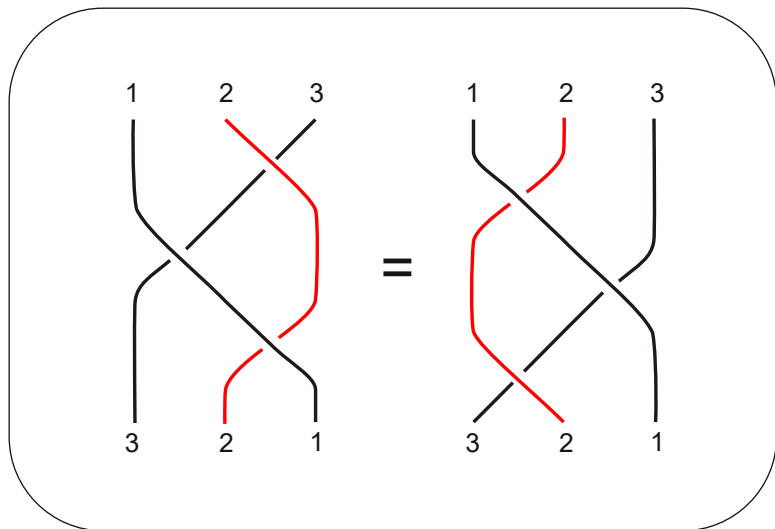


$$= \sigma_j$$



$$= \sigma_j^{-1}$$

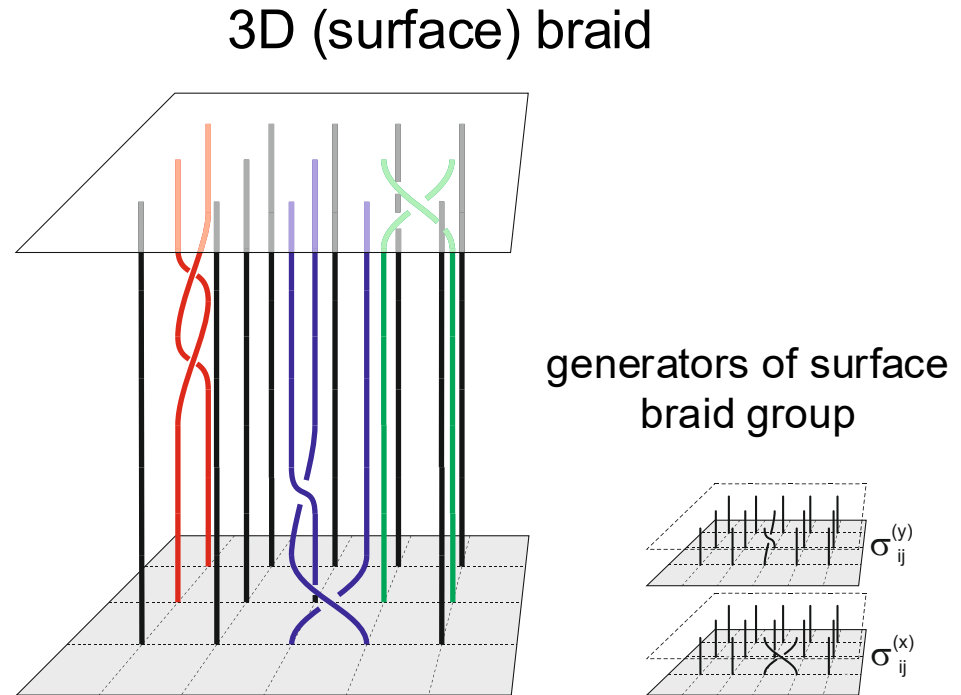
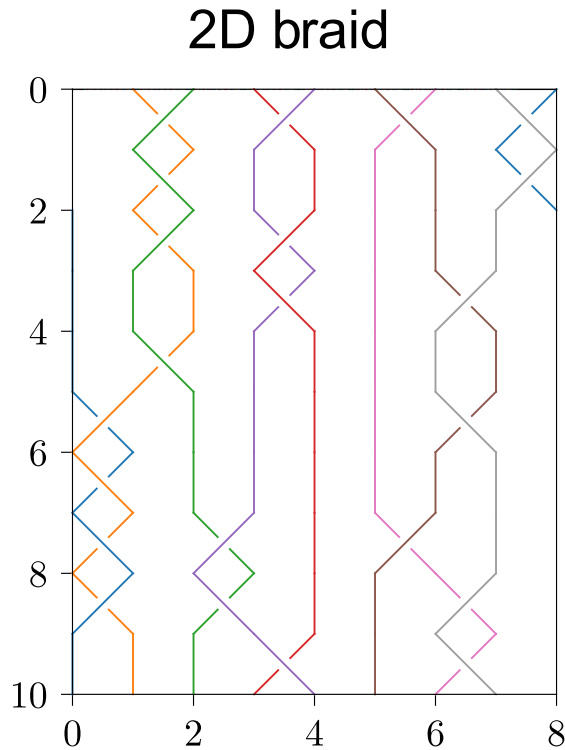
generators of braid group B_n



braid group relations

$$\begin{cases} \sigma_j \sigma_{j+1} \sigma_j = \sigma_{j+1} \sigma_j \sigma_{j+1} \\ \sigma_j \sigma_k = \sigma_k \sigma_j \end{cases} \quad |k - j| \geq 1$$

Typical examples of 2D- and 3D-braids

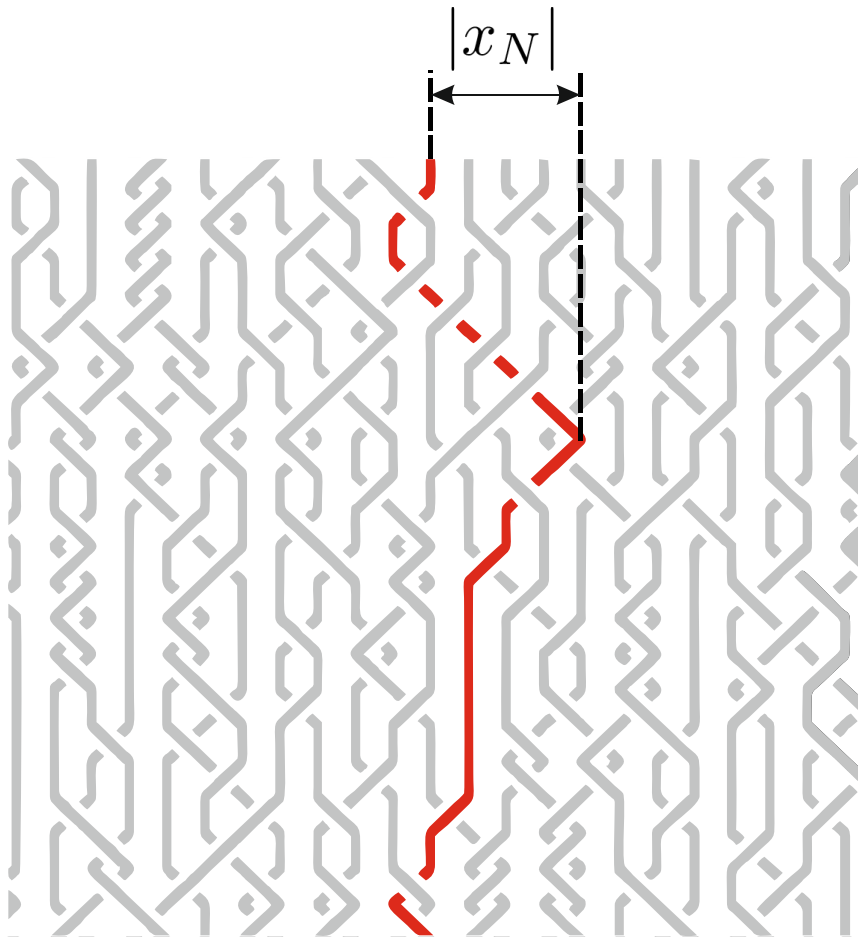


Identifying upper and lower ends of directed polymers (threads) we get a collection of mutually entangled loops

Random braid is obtained by assuming some distribution on the set of generators $\{\sigma_1, \dots, \sigma_n, \sigma_1^{-1}, \dots, \sigma_n^{-1}\}$.

Anomalous fluctuations of threads in trivial braids

Consider uniform distribution on the set $\{\sigma_1, \dots, \sigma_n, \sigma_1^{-1}, \dots, \sigma_n^{-1}\}$ and demand *the braid to be trivial*, i.e. each thread is not entangled with all others. Such a braid is *topologically* equivalent to the set of parallel lines. We are interested in the mean transversal span of threads in *subset of random trivial braids*.



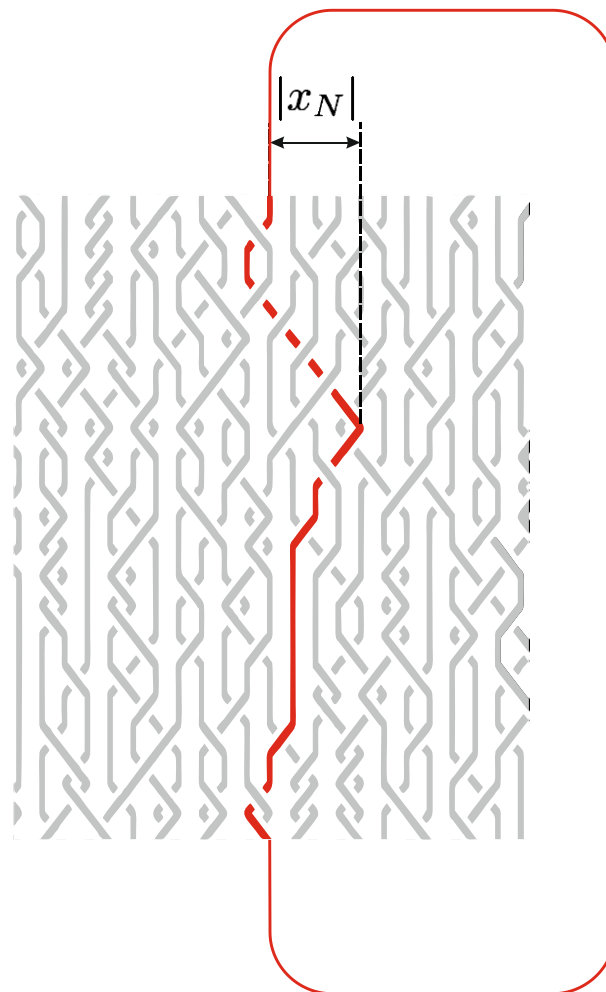
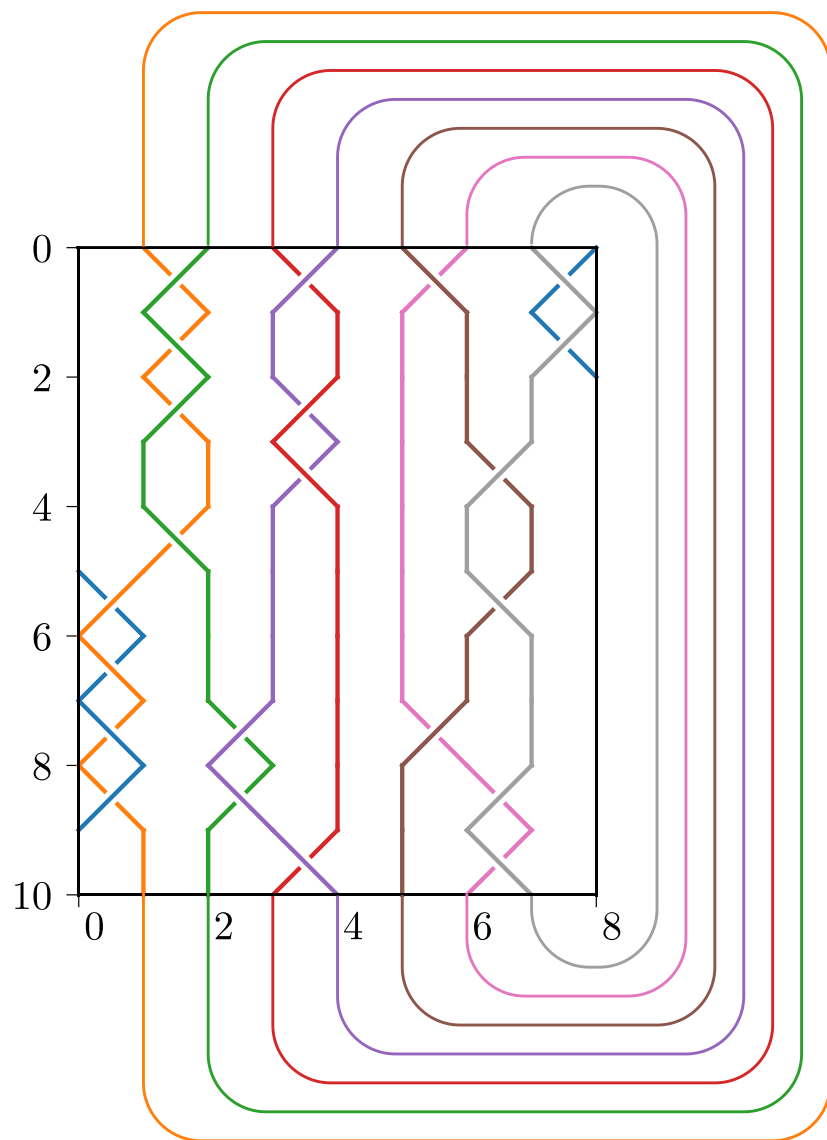
Challenging numerical observation

P. Serna, G. Bunin and A. Nahum, in *Phys. Rev. Lett* (2015), 115, 228303 claimed the asymptotic logarithmic dependence

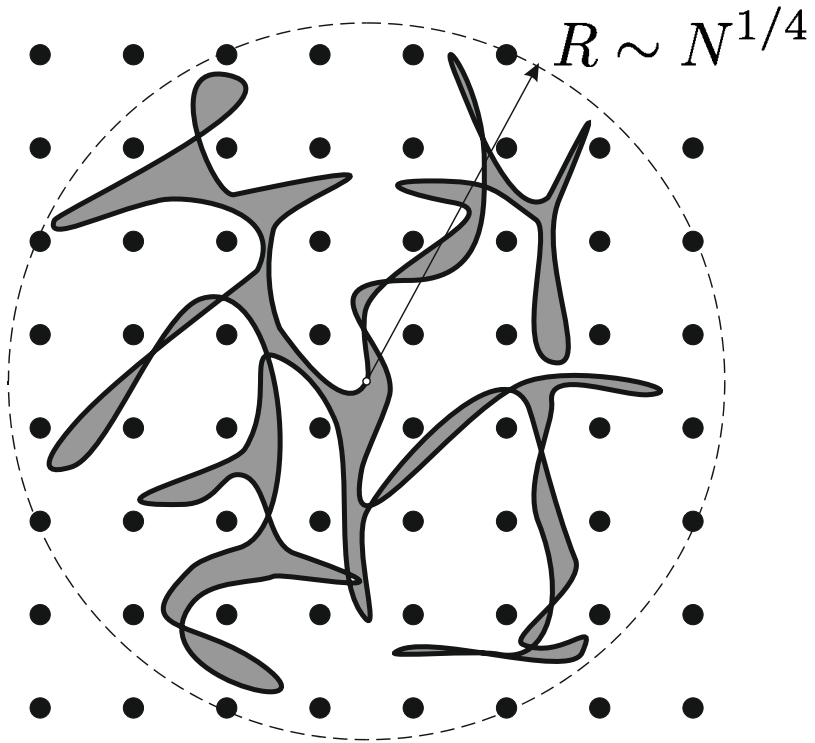
$$|x_N| \sim (\ln N)^\zeta; \quad \zeta \approx 1.49(3)$$

The claim of P. Serna, G. Bunin and A. Nahum contradicts a mean-field-like theory of unentangled random walks in the uniform lattice of obstacles (E. Helfand and D. Pearson, 1983; M. Rubinstein and E. Helfand, 1985; A. Khokhlov and S.N., 1985), which should give

$$|x_N| \sim N^{1/4}$$



Reference model: Unentangled loop in a lattice of obstacles

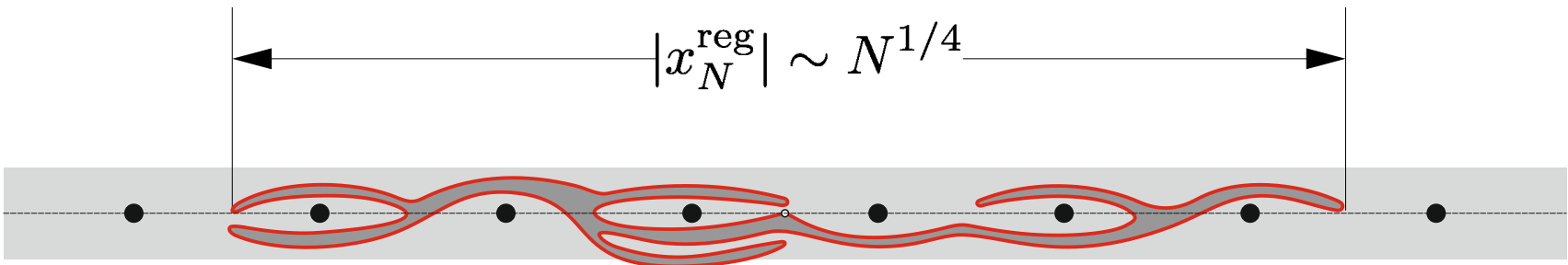


Typical size of a random loop
("Brownian bridge") on a uniform tree

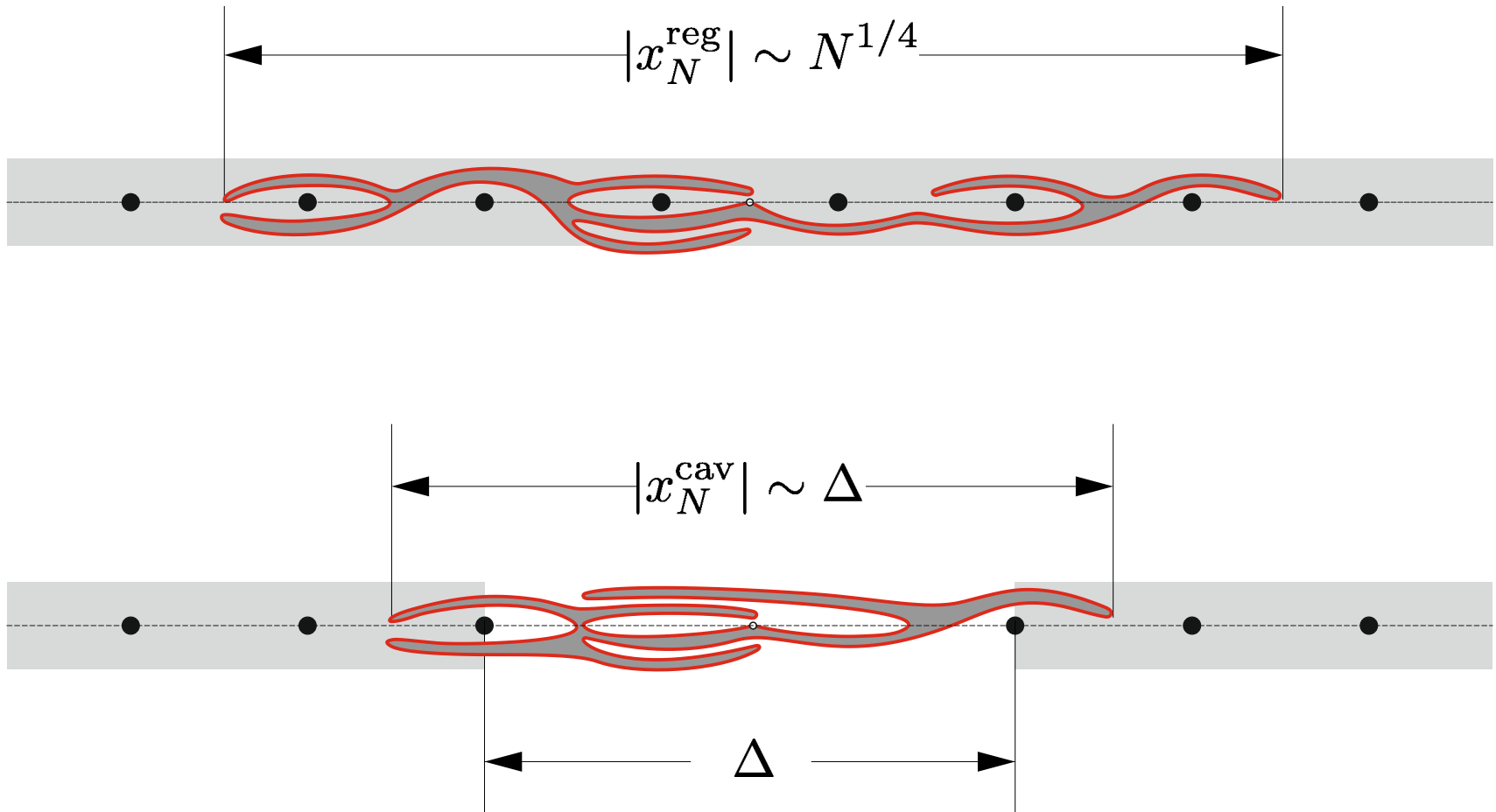
$$l \sim \sqrt{N}$$

Distances on the tree randomly fluctuate
in space, and have typical spatial size

$$|x_N| \sim \sqrt{l} \sim N^{1/4}$$



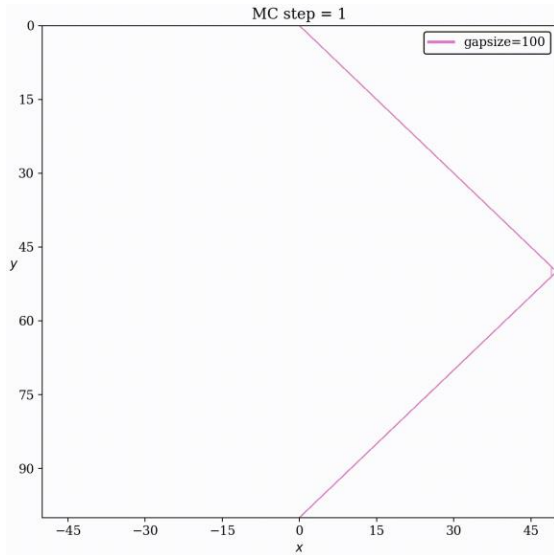
Unentangled loop in a lattice of obstacles with a cavity



Unentangled loop is localized on a cavity

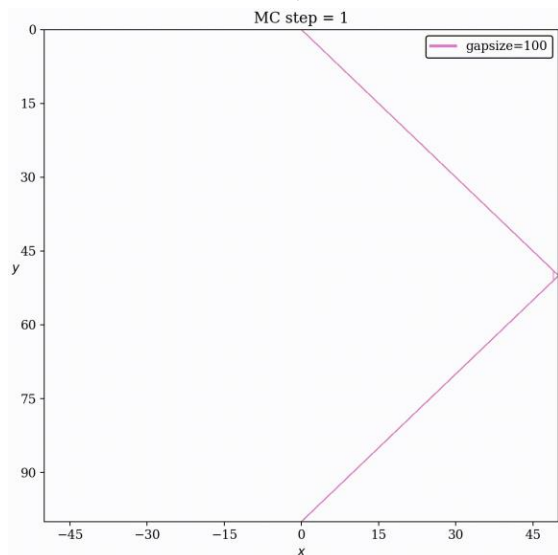
What happens with unentangled paths in the *nonuniform* array of obstacles

Loop on a line without lattice
of obstacles, $\langle |x_N| \rangle \sim N^{1/2}$.

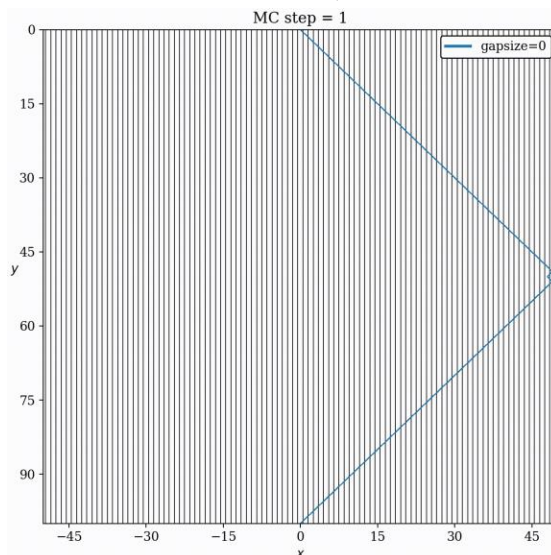


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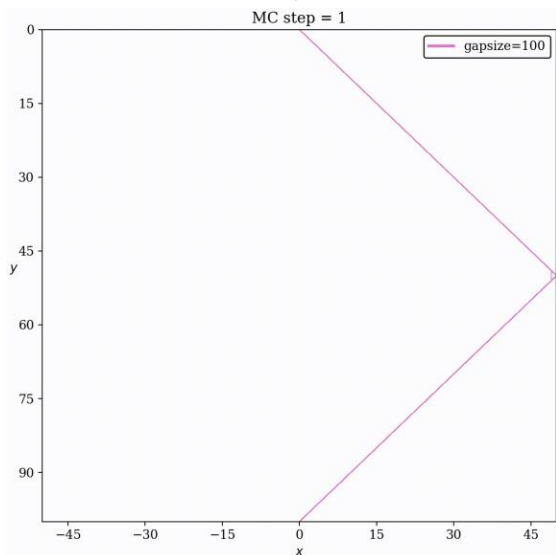


Unentangled loop in uniform lattice of obstacles, $\langle |x_N| \rangle \sim N^{1/4}$.

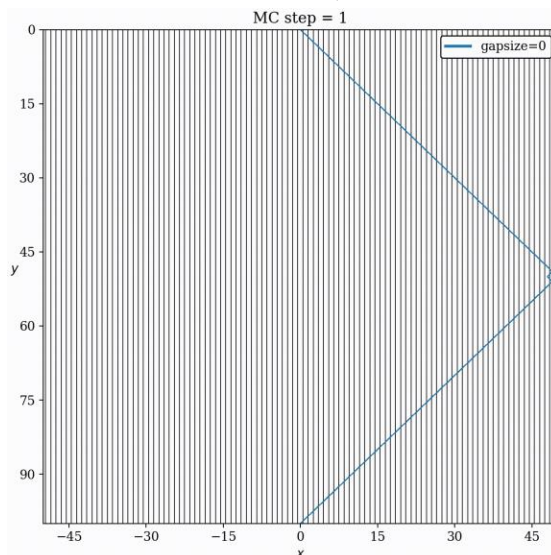


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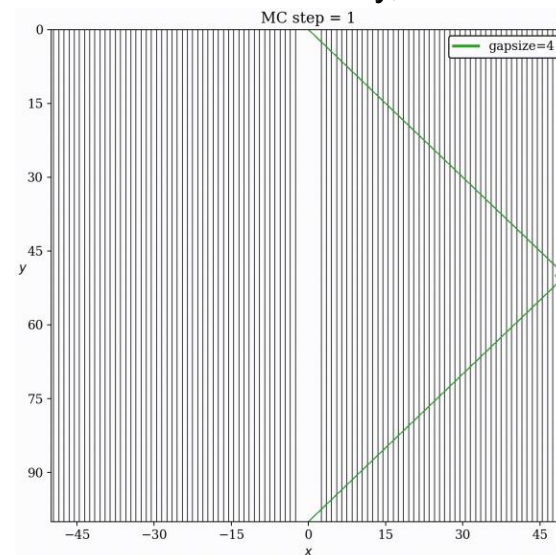
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Unentangled loop in uniform lattice of obstacles, $\langle |x_N| \rangle \sim N^{1/4}$.

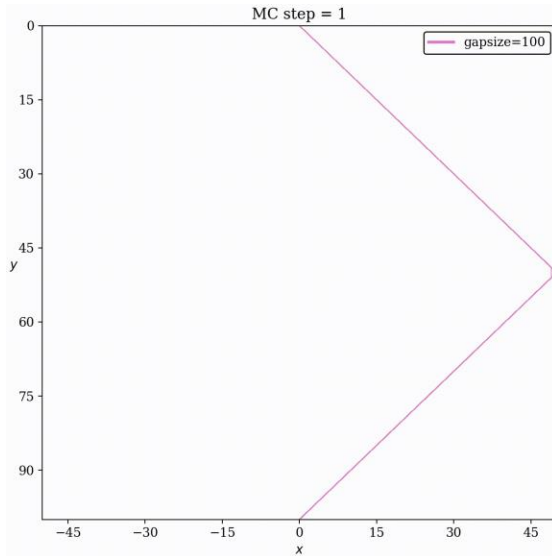


Unentangled loop in array of obstacles with a cavity, $\langle |x_N| \rangle \sim \text{const.}$

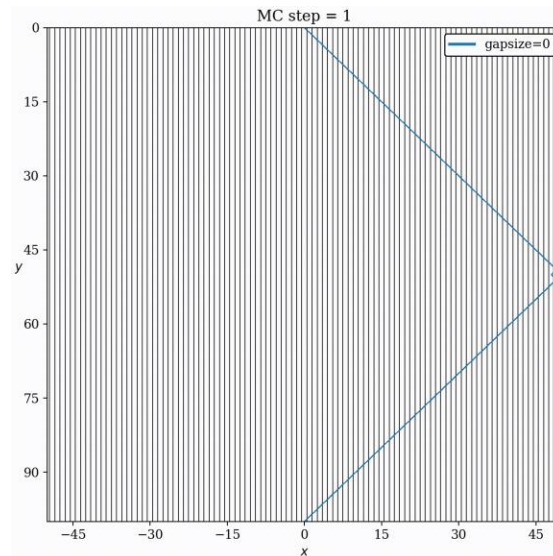


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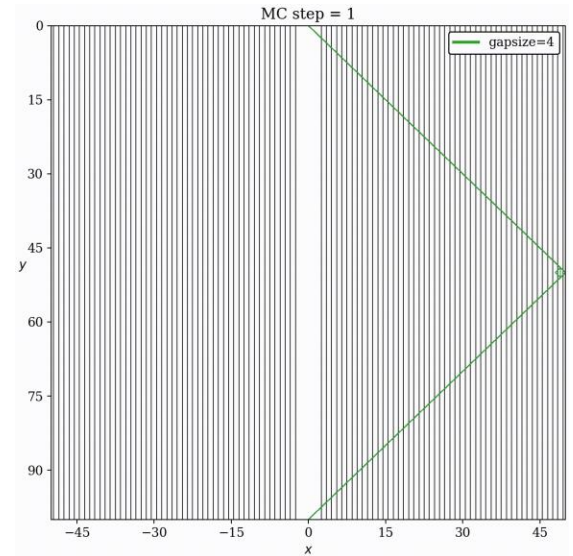
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Unentangled loop in uniform lattice of obstacles, $\langle |x_N| \rangle \sim N^{1/4}$.

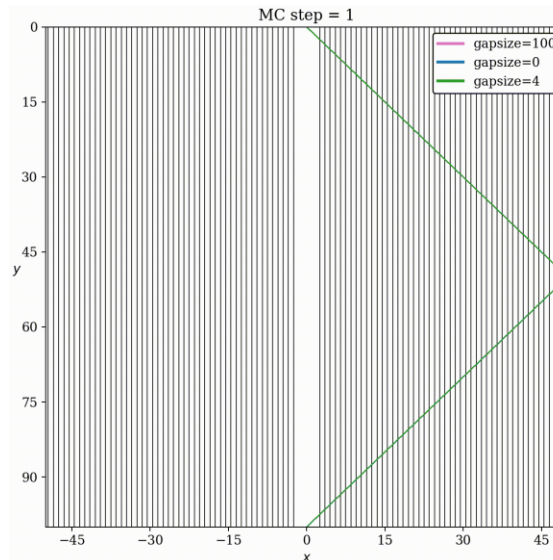


Unentangled loop in array of obstacles with a cavity, $\langle |x_N| \rangle \sim \text{const.}$



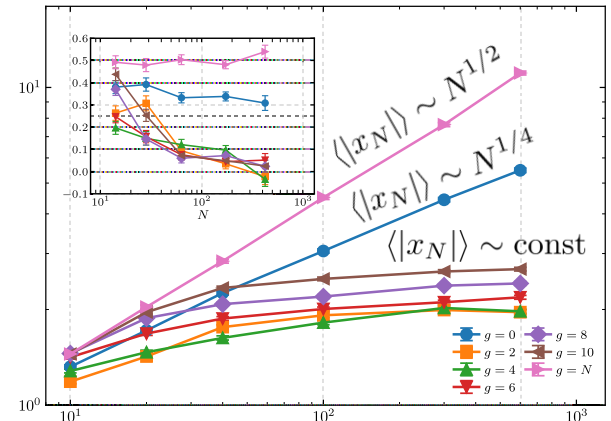
Our main message:

In the nonuniform lattice of obstacles unentangled loop localizes on the cavity free of obstacles



Summary:

Asymptotic behavior of span



Our conjectures (simulations and analytics):

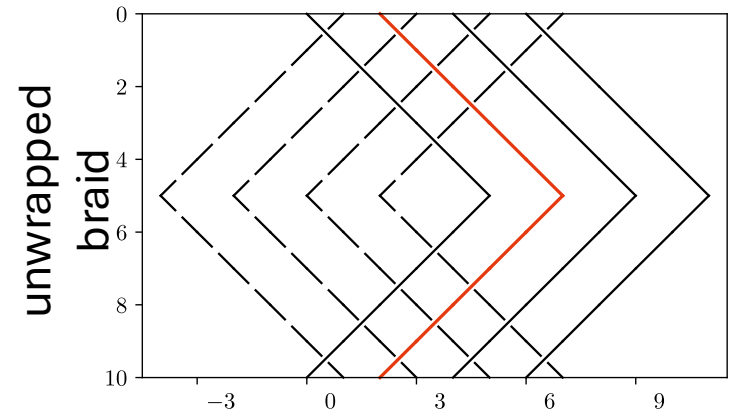
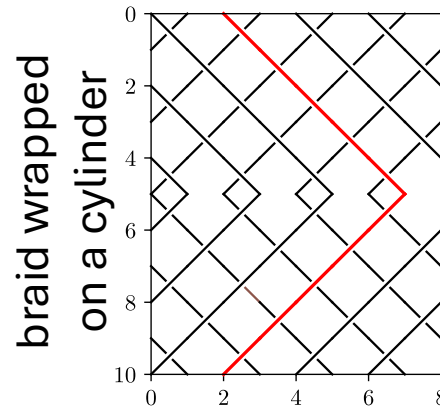
1. Unentangled threads in a braid are *localized* in the transversal direction at $N \gg 1$ for some $n > n_{\text{cr}}$

This statement is stronger than numerical finding of P. Serna, G. Bunin and A. Nahum. We suggest that logarithmic growth of a span is a transient regime for intermediate braid lengths N .

2. There is a delocalization-localization phase transition of threads' transversal fluctuations at $n = n_{\text{cr}}$ for long braids $N \gg 1$

Preparation:

Unentangled fully expanded threads



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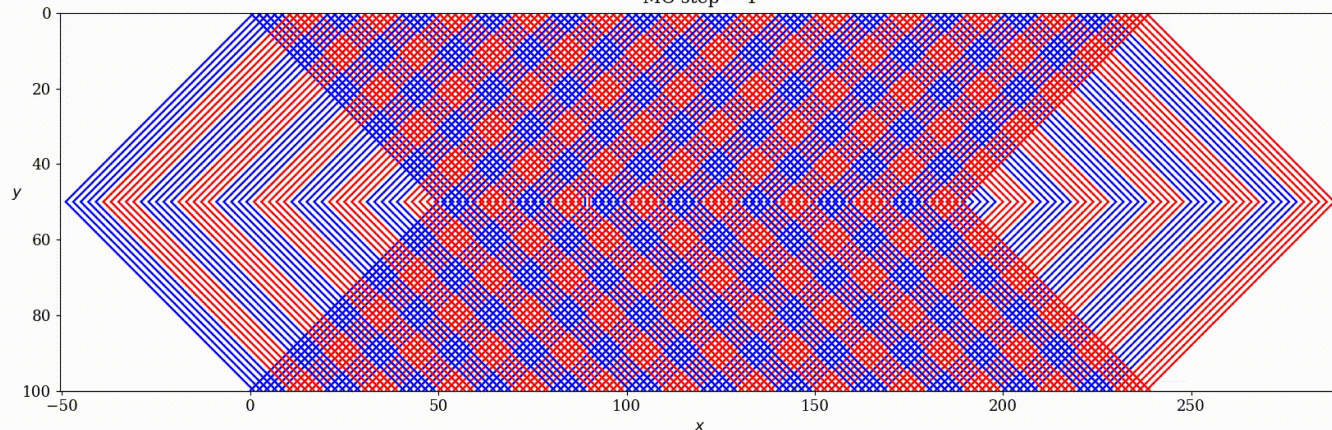
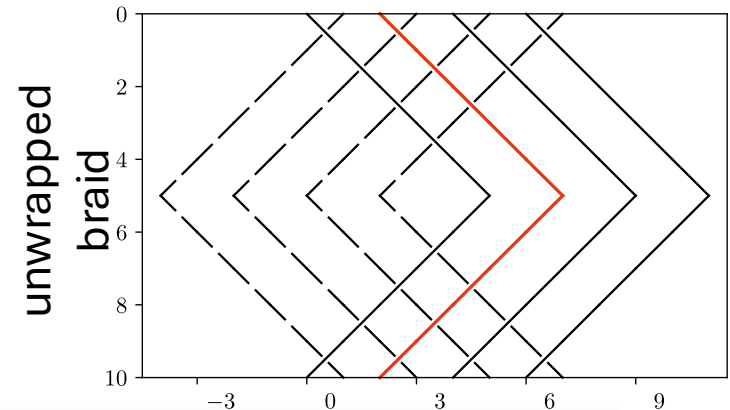
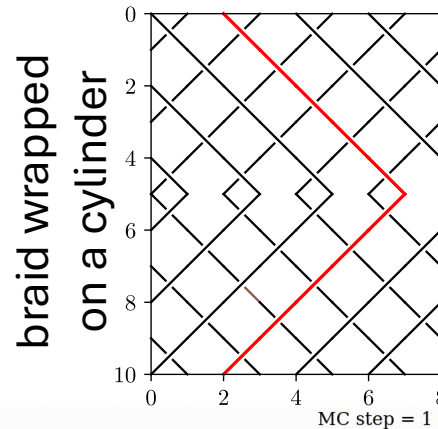
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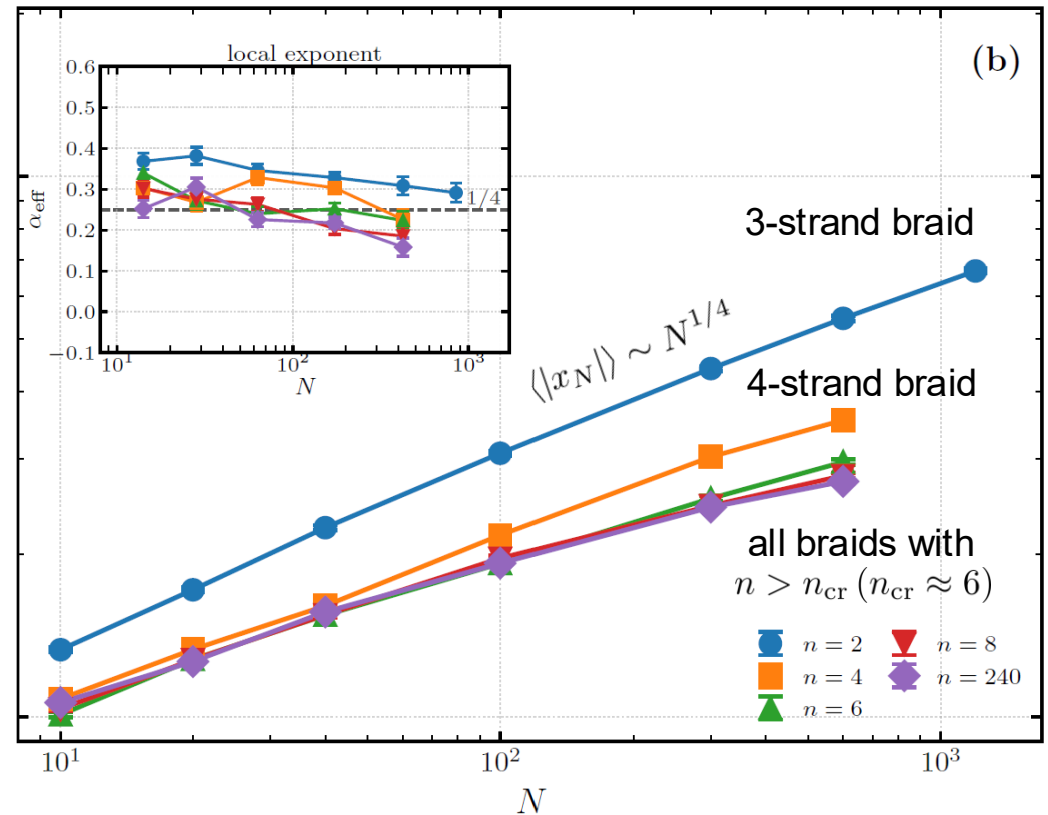
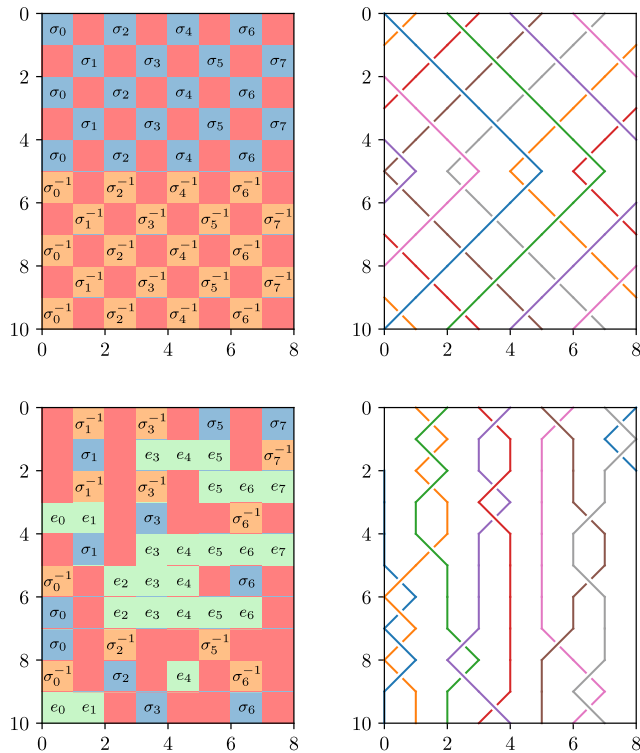
Unentangled fully expanded threads



Algebraic approach to random walk on braid groups

Consider uniform distribution on generators $\{\sigma_1, \dots, \sigma_n, \sigma_1^{-1}, \dots, \sigma_n^{-1}\}$ and write random words of $2N$ letters. Extract subset of such words that are fully contractible. This subset constitutes the ensemble of trivial braids.

We estimate the span of the Brownian bridge (Bb) by the shortest length of the (irreducible) word written by first N letters out of $2N$ -letter Bb.



Braids and locally-free groups

We should understand how the “space of all words” of B_{n+1} looks like, i.e. what is the graph of the braid group B_{n+1} . Then we shall consider statistics of closed random walks (Brownian bridges) on this graph. The span of Bb is defined by the shortest distance along this graph of the middle point of Bb.

Braid graphs are complex objects due to triple relations. We can essentially simplify consideration by approximating braid groups by locally free groups.

Braids are considered in a “*locally-free approximation*” (A. Vershik, S.N., R. Bikbov, *Comm. Math. Phys.*, 2000) where we neglect triple interactions:

Braids, B_{n+1}

Locally-free group, LF_n

$$\begin{cases} \sigma_i \sigma_{i+1} \sigma_i = \sigma_{i+1} \sigma_i \sigma_{i+1} \\ \sigma_i \sigma_j = \sigma_j \sigma_i & |i - j| > 1 \end{cases}$$

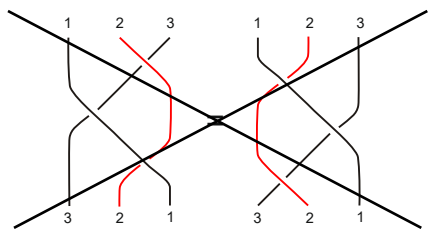
$$\begin{cases} (g_i, g_{i+1}) & \text{do not commute} \\ g_i g_j = g_j g_i & |i - j| > 1 \end{cases}$$

Visualization of generators



Locally free group as approximants of braid group

1. Estimation from above: Number of all *shortest* words of length $2K$ in LF_n denoted as $V(LF_n, 2K)$ gives upper estimate for number of shortest words of length $2K$ in braid group B_{n+1} , $V(B_{n+1}, 2K)$, because B_{n+1} is contained in LF_n due to absence of triple relations:



$$V(B_{n+1}, 2K) \leq V(LF_n, 2K)$$

2. Estimation from below: Number of all *shortest* words of length K in a group LF_n , $V(LF_n, K)$, gives lower estimate for number of shortest words of length $2K$ in braid group B_{n+1} , $V(B_{n+1}, 2K)$, because LF_n is constructed on squares of generators of B_{n+1} :

$$g_i = \sigma_i^2$$

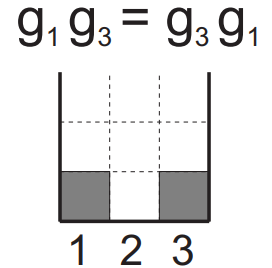
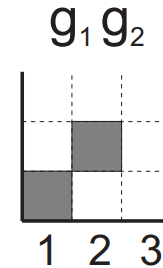
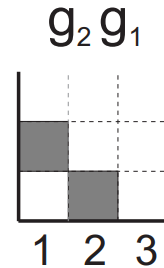
$$V(LF_n, K) \leq V(B_{n+1}, 2K)$$

Hence, we get bilateral estimate for the braid group by locally-free group

$$V(LF_n, K) \leq V(B_{n+1}, 2K) \leq V(LF_n, 2K)$$

Exact word enumeration in the group LF_n and its Cayley graph

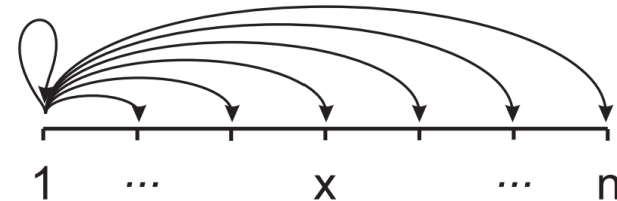
$$g_k g_m = g_m g_k, \quad |k - m| \geq 2.$$



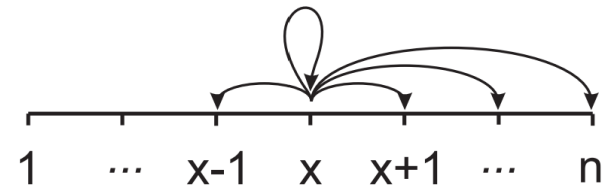
Normal form of a word in LF_n : $W = (g_{\alpha_1})^{m_1} (g_{\alpha_2})^{m_2} \dots (g_{\alpha_s})^{m_s}$

where $\sum_{i=1}^s |m_i| = K$ ($m_i \neq 0 \forall i; 1 \leq s \leq K$) and $\alpha_1, \dots, \alpha_s$ satisfy the conditions:

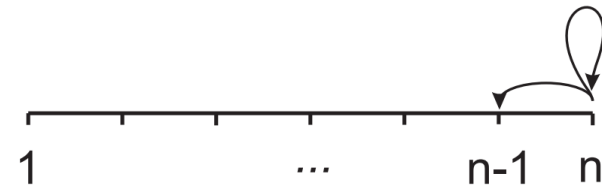
(i) If $\alpha_i = 1$ then $\alpha_{i+1} = 2, \dots, n$;



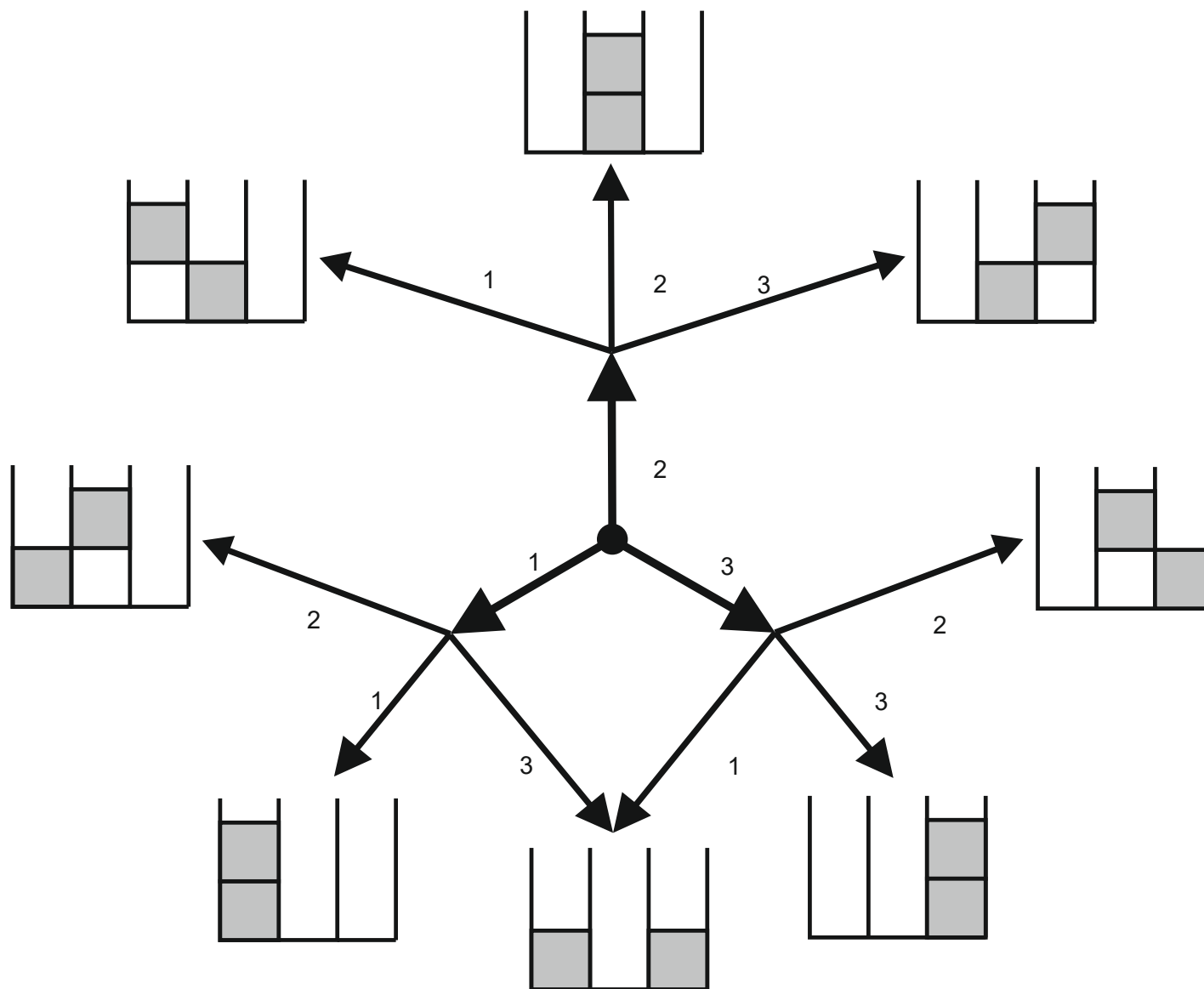
(ii) If $\alpha_i = k$ ($2 \leq k \leq n-1$) then
 $\alpha_{i+1} = k-1, k+1, \dots, n$;



(iii) If $\alpha_i = n$ then $\alpha_{i+1} = n-1$.

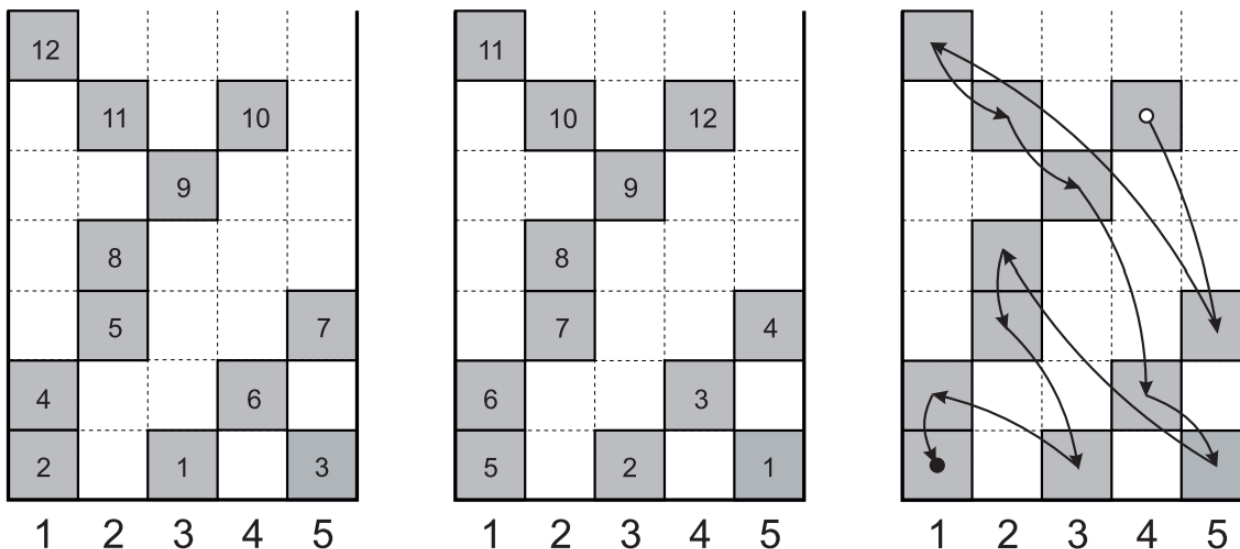


Exact word enumeration in the group LF_n and its Cayley graph

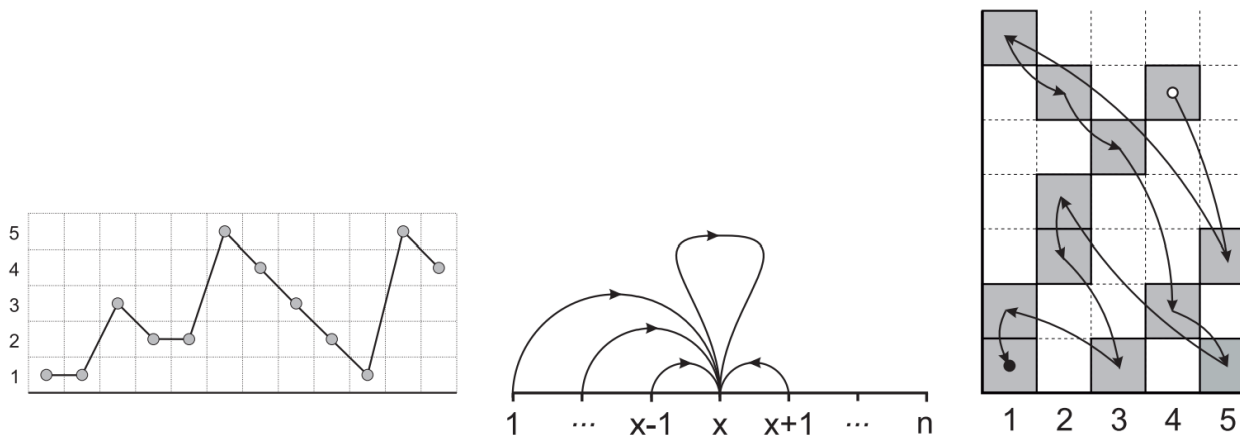


Words as heaps of pieces

“Mikado” algorithm of enumeration of words



Equivalent descriptions: Lukasiewicz paths and Mikado ordering



The numbers of topologically different heaps, $Z_N(x, x_0|n)$, which defines the number of different words (different classes of equivalences in the semigroup of positive generators) satisfies the recursion relation

$$\begin{cases} Z_{N+1}(x, x_0|n) = \sum_{x'=1}^{x+1} Z_N(x', x_0|n), & x = 1, \dots, n; \\ Z_{N=0}(x, x_0|n) = \delta_{x, x_0} \end{cases}$$

It is convenient to rewrite this recursion in a matrix form

$$Z_N(x, x_0|n) = \langle \mathbf{X}_{out} | T^N(n) | \mathbf{X}_{in} \rangle;$$

$$\mathbf{X}_{in} = (\overbrace{0, \dots, 0}^{x_0}, 1, 0, \dots, 0)^\top, \quad \mathbf{X}_{out} = (\overbrace{0, \dots, 0}^x, 1, 0, \dots, 0)$$

where the matrix $T(n)$ is the transfer matrix of Lukasiewicz paths:

$$T(n) = \begin{pmatrix} 1 & 1 & 1 & 1 & \dots & 1 \\ 1 & 1 & 1 & 1 & \dots & 1 \\ 0 & 1 & 1 & 1 & \dots & 1 \\ 0 & 0 & 1 & 1 & \dots & 1 \\ \vdots & \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \dots & 1 \end{pmatrix}$$

The growth rate, $\Lambda(n)$, of a heap is determined by the largest eigenvalue of the transfer matrix, $T(n)$:

$$\Lambda(n) = 4 \cos^2 \frac{\pi}{n+1} \Big|_{n \gg 1} \approx 4 - \frac{4\pi^2}{n^2}$$

Thus, in a large bounding box of base $n \gg 1$ the growth rate is saturated at the value

$$\lambda_\infty = \lim_{n \rightarrow \infty} \Lambda(n) = 4$$

Let us recall that geometric heaps correspond to enumeration of words in a semigroup, LF_n^+ , constructed in terms of generators g_i in positive powers only. Number of pieces in a heap, N , equals to the length of shortest word, k .

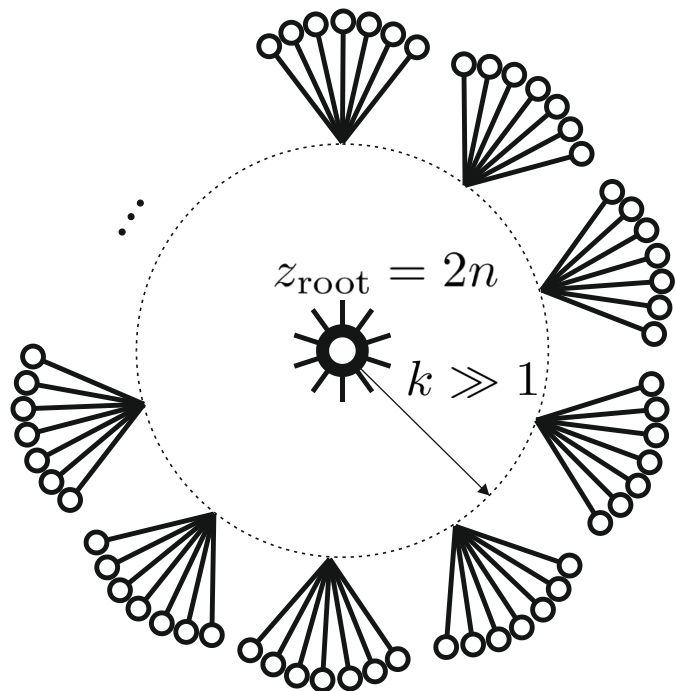
The number of classes of equivalences, $Z_N^{\text{full}}(n)$, in the full locally-free group, LF_n , can be exactly computed taking into account multiplicity of indices. The logarithmic volume of the group LF_n grows as

$$v = \lim_{k \rightarrow \infty} \lim_{n \rightarrow \infty} \frac{\ln Z_k^{\text{full}}(n)}{k} = \ln 7$$

The fact that $v = \ln 7 = \text{const} > 0$ indicates that on large distances from the root point, $k \gg 1$, the graph of the locally free group LF_n (and hence of the braid group B_{n+1}) grows not faster than the **effective Cayley tree with $z_\infty^{\text{out}} = 7$ outer branches**:

$$z_\infty^{\text{out}} = 3 + 4 \cos \frac{2\pi}{n} \Big|_{n \gg 1} \approx 7 - \frac{8\pi^2}{n^2} \Big|_{n \rightarrow \infty} \rightarrow 7$$

...while at the root point the number of branches is unbound.

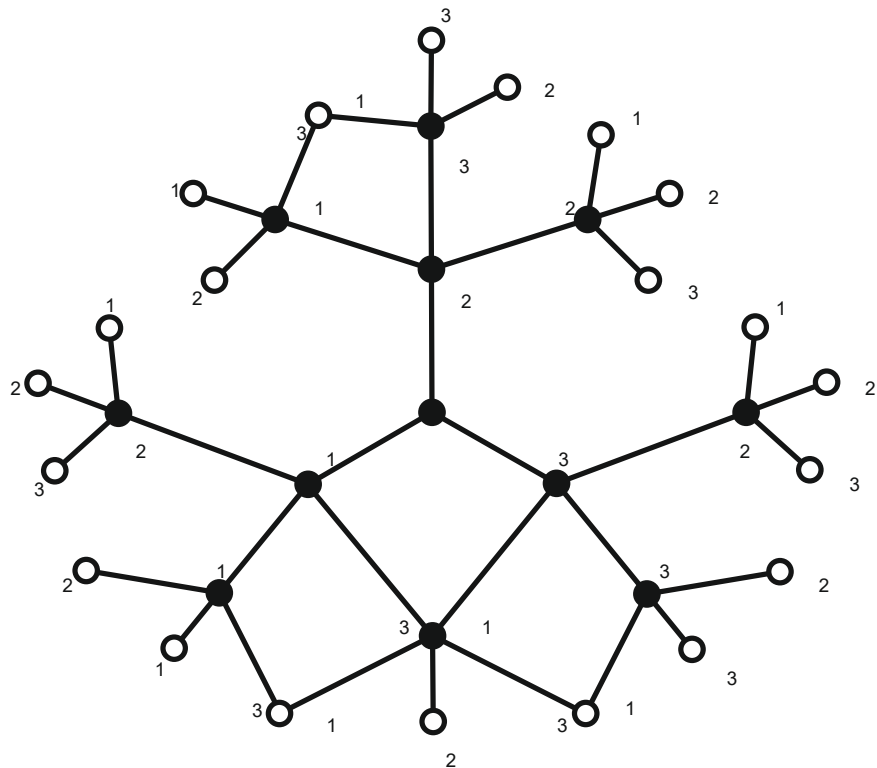


Conjecture

The graph of the locally-free group at large n looks asymptotically as an **effective tree with a heavy root** where n is the control parameter.

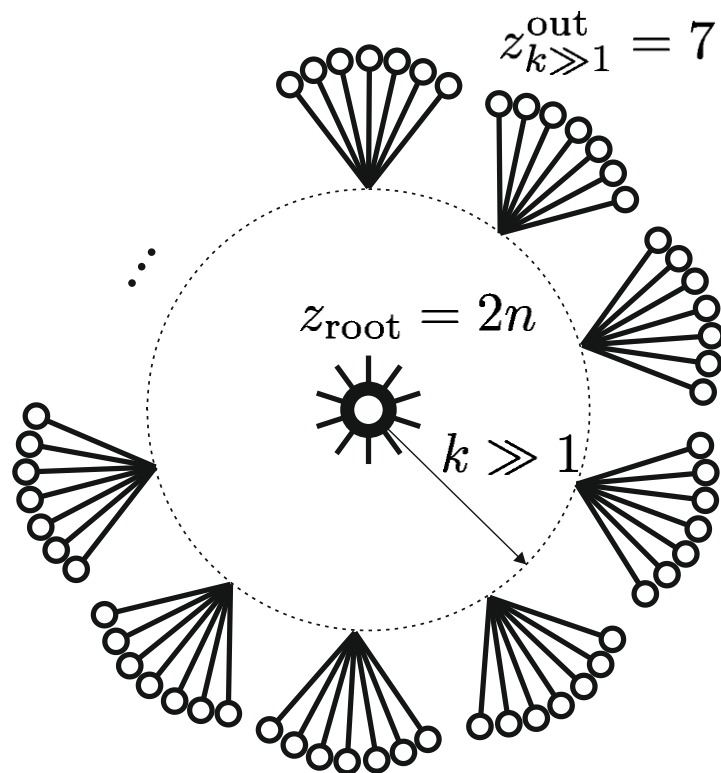
$$z_\infty = 8 = 7(\text{out}) + 1(\text{in})$$

Graph of
semigroup LF_3^+



(a)

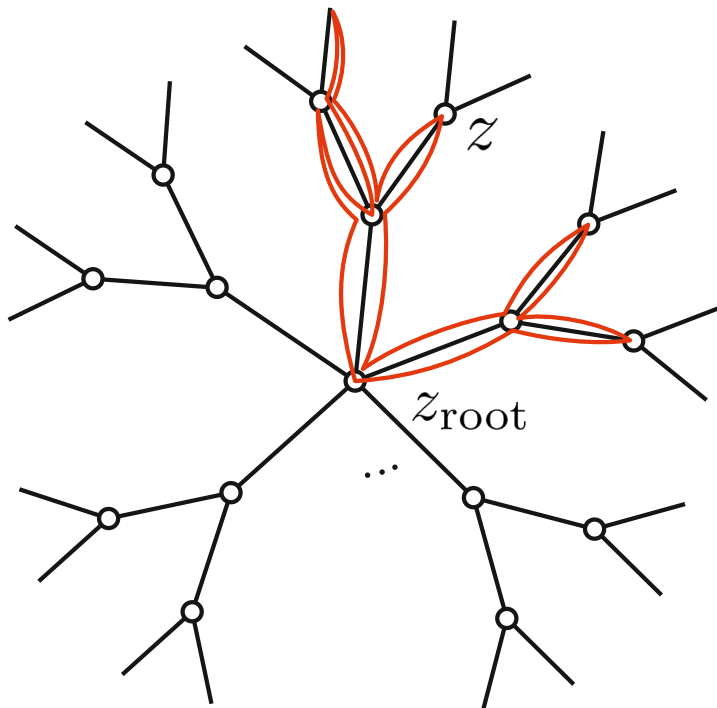
Effective asymptotic graph
of group $LF_n|_{n \gg 1}$



(b)

Analytic arguments in support of threads' localization

1. Random loops on an uniform tree with a “heavy root”



Loops localize at the heavy root by the 2nd order phase transition at the critical point

$$z_{\text{root}} = 2(z - 1)$$

- At $z_{\text{root}} < 2(z - 1)$ the loop has typical span $l \sim N^{1/2}$ on the tree;
- At $z_{\text{root}} > 2(z - 1)$ the loop is localized in the vicinity of the root and has a typical span $l \sim \text{const}$ on the tree.

The localization mechanism is purely entropic:

At sufficiently large values of z_{root} and fixed z the configurational entropy of the root exceeds the entropy of configurations expanded over the tree.

Analytic arguments in support of threads' localization

2. Localization of loops on an asymptotic graph of a locally-free group

- a) Trivial braid (all threads are unentangled) = loop (Brownian bridge) on the graph of a locally-free group
- b) The graph of the locally free group on large distances $k \gg 1$ and for $n \gg 1$ looks is an effective tree with $z_{\infty}^{\text{out}} = 7$ outer branches but the root point is “heavy” with $z_{\text{root}} = 2n$ branches.

Thus, we can apply the above discussion of “entropic localization” of loops at the origin of a tree-like graph with a heavy root, which support the following statement:

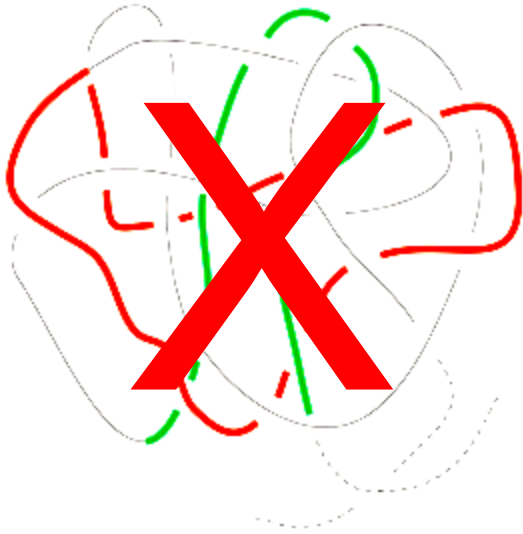
There is a critical n_{cr} such that for $n > n_{\text{cr}}$ the Brownian bridges on the braid group (i.e. unentangled paths) are localized in the finite layer at the root point of the graph of the group.

Summary:

Collective mechanism behind spontaneous localization

- Transverse moves change topological accessibility of neighboring threads, opening “gates” (holes), which provide further spontaneous localization of an unentangled chain in an effective inhomogeneous array of obstacles;
- Consequently, localization of one chain generates a hole for other chains and hence is the nucleus producing avalanche of instabilities resulting in emergent microphase segregation in unentangled threads.
- Algebraically, statistics of random entanglements of threads can be viewed as a random walk on the braid group. Return to the origin (Brownian bridge) means complete disentanglement of all threads. On large scales the graph of the braid group looks as a tree with a “heavy root” which favors localization of Brownian bridges.
- Found behavior could have important consequences for understanding the roughness of boundaries between chromosomal territories.

How can a linear chain be tightly packed in space so that each part would be (almost) unknotted?

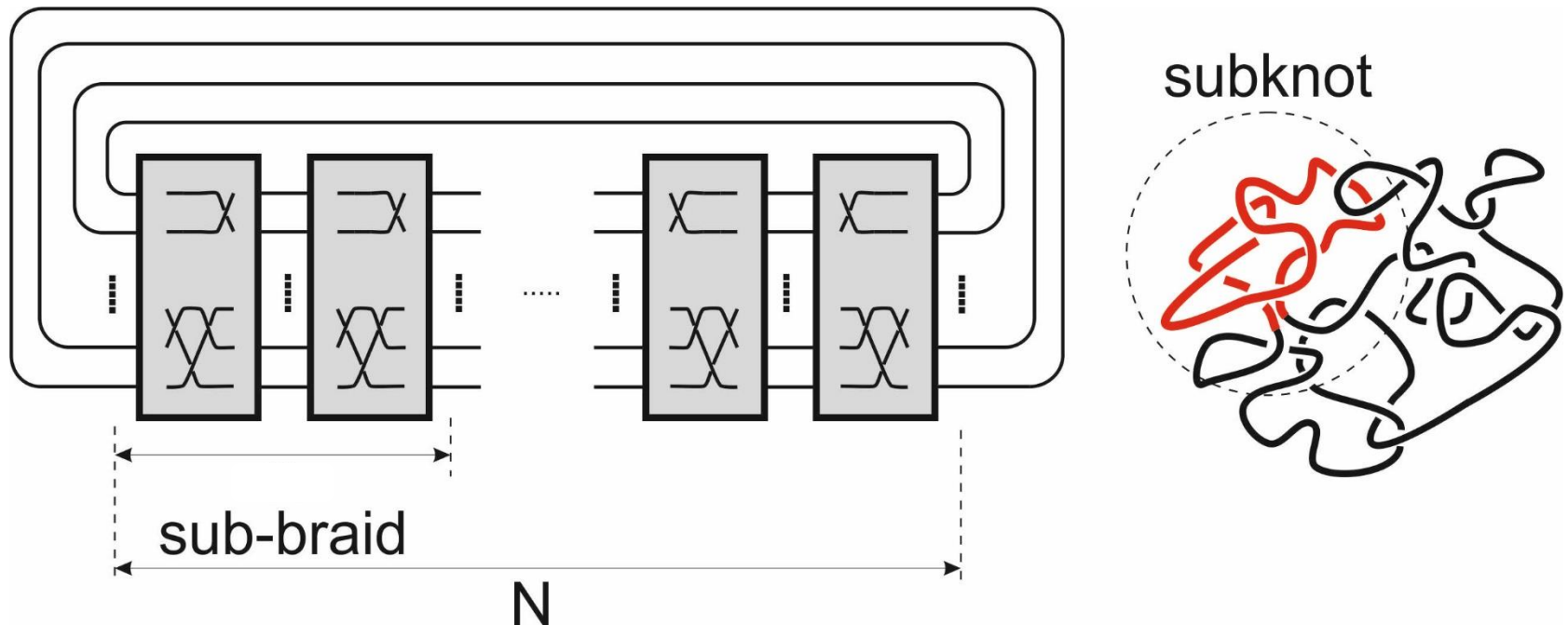


Different chain parts
penetrate into each other
forming quasi-entanglements



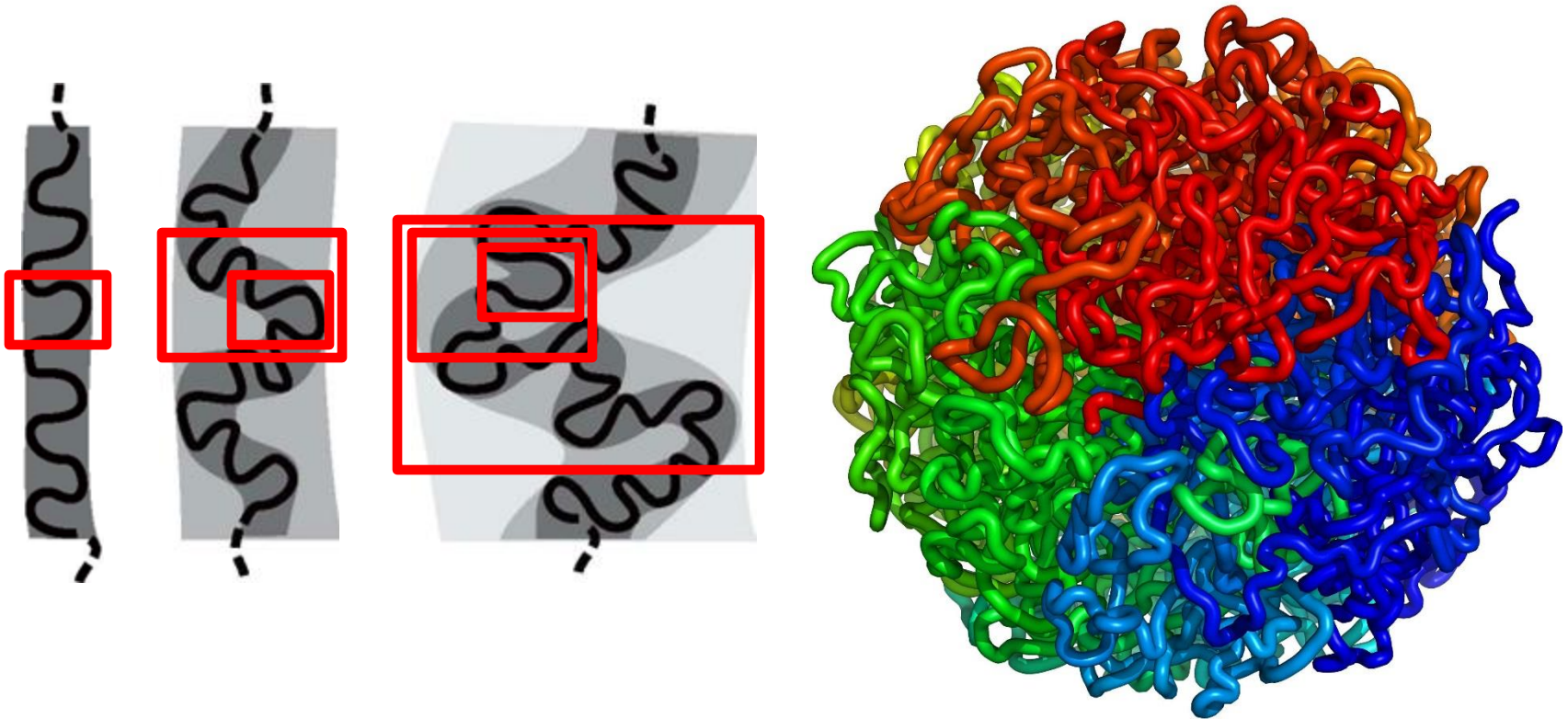
Neighboring monomers *along a chain* are mostly neighbors *in space* and are weakly entangled

How can a linear chain be tightly packed in space so that each part would be (almost) unknotted?



M. Imakaev, K. Tchourine, S.N., L. Mirny (Soft Matter, 2014)

How can a linear chain be tightly packed in space so that each part would be (almost) unknotted?



Chain is continuously painted in **rainbow** colors from one end to the other.
“Territorial structure” shows that monomers neighboring along a path are
neighboring in space